JOURNAL OF VACUUM SCIENCE AND TECHNOLOGY A

Lattice curvature of InxGa1−xAs/GaAs [001] graded buffer layers

F. Romanato, M. Natali, E. Napolitani, A. V. Drigo, A. Bosacchi et al.

Citation: J. Vac. Sci. Technol. A **16**, 3578 (1998); doi: 10.1116/1.581001
View online: http://dx.doi.org/10.1116/1.581001
View Table of Contents: http://avspublications.org/resource/1/JVTAD6/v16/i6
Published by the AVS: Science & Technology of Materials, Interfaces, and Processing

This section is reserved for short submissions which contain important new results and are intended for accelerated publication.

Lattice curvature of $In_xGa_{1-x}As$/GaAs [001] graded buffer layers

F. Romanato,[a)] M. Natali, E. Napolitani, and A. V. Drigo
Istituto Nazionale Fisica della Materia (INFM)—c/o Dip. di Fisica ''Galileo Galilei'' via Marzolo 8, I-35131 Padova, Italy

A. Bosacchi, C. Ferrari, S. Franchi, and G. Salviati
Instituto Materiali Speciali (MASPEC-CNR) via Chiavari 18A, 43100 Parma, Italy

(Received 23 April 1998; accepted 31 July 1998)

Ion channeling analysis and x-ray diffraction reciprocal space maps have been performed on $In_xGa_{1-x}As$ buffer layers grown with different composition profiles on well-cut (001) GaAs substrates. On all of the samples analyzed we detect a *curvature* of the layer lattice, i.e., a tilt of the lattice with respect to the substrate which varies coherently along the sample surface. The layer tilt is directed inward defining a curvature that is concave, large (up to 2.5° cm^{-1}) and that decreases when approaching the substrate. We describe this new phenomenon in terms of a coherent lateral distribution of the orientations of the misfit dislocation Burgers' vectors. © *1998 American Vacuum Society.* [S0734-2101(98)02506-8]

The growth of optoelectronic grade quality, highly mismatched semiconductor heterostructures on commercially available substrates requires the interposition of suitable buffer layers with controlled lattice parameter. The state of the art is represented by buffer layers with continuous or step-like graded composition profiles. After the seminal works of Fitzgerald[1] and LeGoues[2] and the first model on the depth distribution of misfit dislocations (MD) proposed by Tersoff,[3] many efforts have been spent to improve the control of strain relaxation,[4–9] leading to successful improvements of the electro-optical properties of the over grown active epilayer.[10–12]

Basic to this purpose is a deep comprehension of the mechanisms leading to the formation of the MD. Quite surprising not much interest has been devoted to the epilayer tilt that, on the contrary, can provide important information on the driving force acting on the MDs as testified by the few studies available. Buffer layers grown on substrates off-cut some degrees from the (001) plane have shown large and uniform tilts of the lattice film with respect to substrate, aligned parallel to the off-cut direction.[13] Their origin has been attributed to a preferential nucleation of the MDs with an appropriate vertical component of the Burgers' vectors (BV). By detailed investigation of the tilts as a function of off-cut angle it has been shown that it is possible to extract information on the MD nucleation energy.[14] On the contrary for well-cut (001) substrates small or negligible tilts are expected because of the apparent lack of a BV selective driving force. Nevertheless, some exceptions exist[8,9,15] suggesting that also on well-cut substrates there must be a driving force for the selection of the BVs, which necessarily is different from that proposed in Ref. 14.

In this work we report a new effect concerning the evolution of the tilts on graded buffer layers, grown on well-cut substrates. An investigation of tilts was performed on a set of more than 20 $In_xGa_{1-x}As$ graded buffer layers grown on well oriented (001) GaAs substrates ($\leq 0.1°$ off) with different concentration profiles (continuous with different gradings or step-like with different step height and width). On all of the investigated samples we detected a large coherent variation of the lattice film tilt which depends on the position on the sample surface on a macroscopic scale of several mm. As the substrate curvature detected is null, we are dealing only with a *film curvature*. The plastic origin of the phenomenon has been described on the basis of a lateral distribution of the Burgers' vectors whose macroscopic spatial coherence opens new perspectives for the investigation of the mechanisms of strain relaxation.

The main features of the phenomenon are described showing the results concerning two of the most representative samples investigated: one with the compositional profile divided into six equal steps (SB), the other linearly graded (LB). The composition profiles of SB and LB have the same total thickness ($t_b = 2.4\ \mu m$) and final In atomic concentration ($x_b = 0.35$). The samples were grown by molecular beam epitaxy using an As_4 beam at 500 °C with a beam-equivalent pressure (BEP) of 5.5×10^{-6} Torr, while the As_4/Ga BEP ratio was ~9. During the growth they were kept in rotation to maximize the uniformity over the surface ($16\times13\ mm^2$).

Rutherford backscattering spectrometry (RBS) analysis in channeling condition was performed using a $^4He^+$ beam de-

[a)]Present address: INFM at ELETTRA Synchrotron Light Source in AREA Science Park, Strada Statale 14—Km. 163.5, 34012, Basovizza, Trieste, Italy; electronic mail: romanato@sci.area.trieste.it

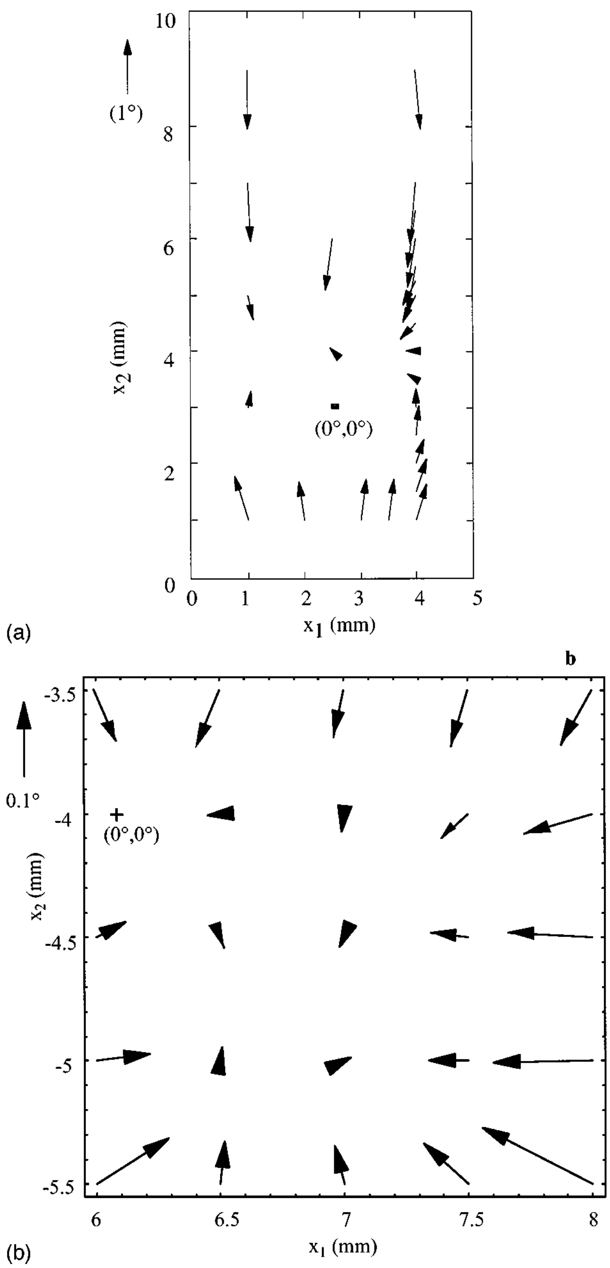

FIG. 1. Maps of the [001] axis direction on the surface of step-like (a) and linear (b) compositionally graded buffer layers. Each position probed on the sample surface corresponds to an arrow representing the angular deviation of the [001] axis direction with respect to the reference direction (+). The components of these arrows give the magnitude of the lattice tilt along the ⟨110⟩ directions which can be compared to the marker.

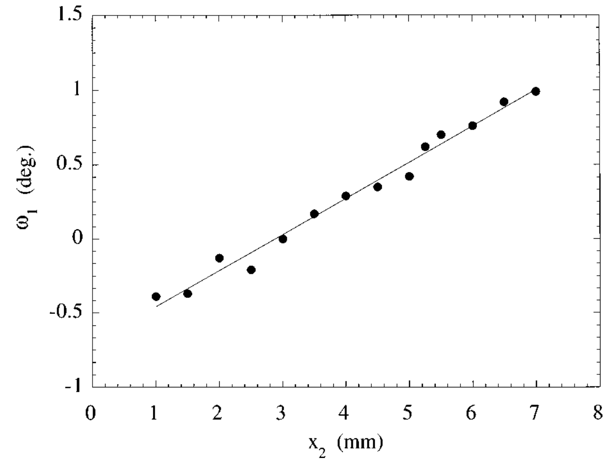

FIG. 2. Tilt angles of sample SB as a function of the position. The tilts around $x_1=[1\bar{1}0]$ of Fig. 1(a) at $x_1=4$ mm are plotted vs x_2.

livered by the 2 MV Van der Graaff accelerator at National Laboratories of Legnaro (Italy). The channeling angular coordinates of the [001] axis were determined by means of a goniometer (0.01° precision) mapping the sample surface typically over areas of several tens of mm^2, with a lateral resolution fixed by the beam spot diameter (0.5 mm).[16] The data of SB and LB have been elaborated as maps of deviation of the epilayer [001] direction relative to an arbitrary reference direction (Fig. 1). Although the RBS-channeling technique can probe several microns of thickness, the channeling analysis of the tilt must be limited to the topmost region of the epilayer free of MDs ($\simeq 100$ nm). In fact, the trajectories of the channeled ions are steered by the epilayer lattice and therefore constrained to follow the depth evolution of the epilayer deformation. As a consequence, one cannot measure the lattice orientation of the deeper regions.[17] This is also the reason why the signal from the substrate cannot be used as a reference and an arbitrary reference direction has been chosen for the channeling maps. However, in order to measure the substrate curvature by channeling technique it is possible to bypass the limitation of the steering effect repeating the analysis on the back of the samples. A negligible ($\leqslant 0.1°$/cm) substrate curvature has always been observed.

The buried regions of the buffer layers were investigated by recording x-ray reciprocal space maps (RSM) around the (004) and (335) reflections with a triple-axis-diffractometer at BM05 of ESRF (Grenoble, France). The bending magnet synchrotron radiation was monochromatized at a wavelength of 1.49976 Å by a Si(111) crystal and then collimated by means of slits on the sample surface producing a spot of footprint 1×1 mm^2. The RSMs were recorded using a NaI scintillator counter prefaced by a Si(111) two-bounce analyzer crystal. Rocking curves of the (004) substrate peak recorded at different positions on the sample surface confirmed the absence of substrate curvature.

We summarize the main features of the phenomenon describing the results of the analysis of LB and SB.

(a) *Lateral dependence of tilt.* Figures 1(a) and 1(b) show a continuous and monotonic variation of tilt on a scale of several mm (i.e., of the same order of magnitude of the sample size). The position dependence of the tilt defines a concave curvature of the film lattice (arrows inward directed) that is opposite to what would be expected for a pseudomorphic film+substrate system under compression (convex curvature). By defining the frame of reference, $x_1=[1\bar{1}0]$, $x_2=[110]$, $x_3=[001]$, Fig. 2 shows that the tilt ω_1 measured on SB around the x_1 axis has a nearly linear dependence on

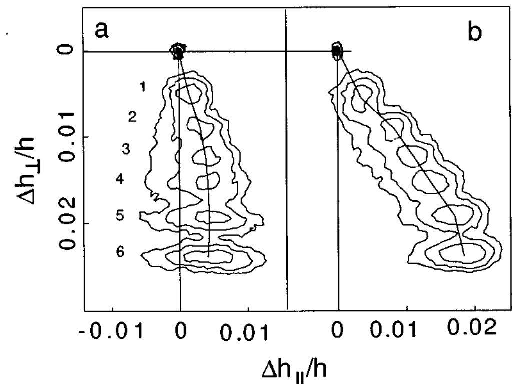

FIG. 3. Maps around the (004) point of reciprocal space collected at the reference point (Fig. 1) of the SB sample (a) and 3 mm away (b).

the lateral coordinate x_2. The curvature along [110], $\partial\omega_1/\partial x_2$, is constant and amounts to 2.4° cm. A concave, nearly constant, curvature was observed also on all of the other samples with values ranging from 0.5 to 2.8° cm.

(b) *The symmetry of the curvature depends on the composition profile.* A comparison of Figs. 1(a) and 1(b) clearly shows that the curvature is present along both the x_1 and x_2 axes in LB while it develops preferentially along the [110] direction in SB. This difference is a general feature that we always observed distinguishing continuously from step graded buffer layers.

(c) *Depth dependence.* Figure 3 shows the RSMs collected at different positions on the surface of SB. A comparison of the peak positions [Figs. 3(a) and 3(b)] confirms that the parallel component of the scattering vector, $h_\parallel$, which is proportional to the tilt, changes with the position of the beam spot on the surface [see item (a)]. Here we want to stress mainly that it also increases with the ordinal number of the layer (nearly proportionally), showing that the curvature starts at the interface with the substrate and increases at each interface (Table I).

From these results it clearly appears that we are not dealing with a simple bending of the whole film+substrate system but, instead, with a coherent variation of the layer tilt which thus defines a *film curvature*.

It is well known that strain relaxation in $In_xGa_{1-x}As$ buffer layers occurs mainly by formation of 60° MDs. In particular, MDs along x_j axis ($j=1,2$) with BV edge components parallel to the interface, b_i ($i=1,2$ $i\neq j$), are responsible for the relaxation of parallel strain along axis x_i. On the contrary, the edge component perpendicular to the interface b_3 is responsible for the film tilt that, in the case of a uniform imbalance, leads to a uniform tilt of the film lattice, $\omega=b_3\,n$, where n is the average density of the MDs.[18] As a consequence, a lateral dependence of the film tilt requires that the average distribution of b_3 depends on position.

TABLE I. Experimental and model [Eq. (2)] values of curvature, $\partial\omega_1/\partial x_2$, of each of six layers (1–6) of SB sample. In Eq. (2) we used $k_1^m=-0.8$, $L=1$ cm, and the reported MDs densities, n_1^m.

Layers		1	2	3	4	5	6
$\partial\omega_1/\partial x_2$	Exp.	0.3	0.8	1.2	1.7	2.1	2.5
(° cm^{-1})	Eq. (2)	0.4	0.8	1.2	1.6	2.0	2.1
n_1^m	(10^4 cm^{-1})	18.8	13.1	18.9	17.4	14.6	4.3

Let us consider the case of the SB. Because the buried layers of SB are almost completely relaxed, the average distance between the MDs at the mth interface parallel to x_j, $1/n_j^m\approx 10-50$ nm, is much shorter than the sample lateral dimension, L. Thus it makes sense to consider a local average of BVs of the MDs parallel to x_j, $\langle\mathbf{b}\rangle_j^m$, performed over a distance $d\approx 10$ μm such that $1/n_j^m\ll d\ll L$. The functional dependence of b_3 can be derived from the analysis of the channeling data that shows that the surface tilt of SB follows a linear dependence on the lateral position (Fig. 2). Then, as a first approximation, the same functional dependence has then been assumed at each interface also for $\langle\mathbf{b}\rangle_j^m$:

$$\langle b_3\rangle_j^m=k_j^m|b_3|\frac{x_i}{L/2}, \quad (1)$$

where $-1\leqslant k_j^m\leqslant 1$ is the parameter qualifying the effectiveness of what we shall call the Burgers vector lateral distribution (BULD). A complete polarization of the BV at the sample edge corresponds to $|k|_j^m=1$; the sign of k_j^m determines the tilt orientation.[19]

The BULD induces at each interface a position dependent tilt between adjacent layers. The total field of rotation comes from the superposition of the fields generated by the networks of MDs at each interface, i.e., the curvature around x_j at the Nth layer of SB results from recurrence of BULD:

$$\frac{\partial\omega_j}{\partial x_i}=\frac{\partial}{\partial x_i}\sum_{m=1}^{N}\langle b_3\rangle_j^m n_j^m=\sum_{m=1}^{N}k_j^m\frac{|b_3|}{L/2}n_j^m. \quad (2)$$

The curvature measured in SB has been compared to the values determined by Eq. (2), evaluating n_j^m (Table I) from the amount of misfit relaxed at each interface.[20] A good agreement can be found using a single value of $k_1^m=-0.8$ for all the layers (Table I). This value implies that almost the maximum efficiency of BULD is required to reproduce the $\partial\omega_1/\partial x_2$ film curvature of SB.

The above description of the curvature in the case of continuously graded profiles can be obtained with a process to the limit by replacing the sum in Eq. (2) with an integral and by considering the depth profile of the MD density. A lower BULD efficiency was found for LB ($k_j^m=-0.3$) and in general for continuous layers.

The observed film curvature cannot be of elastic origin. For a compressive layer a convex curvature of the whole layer+substrate system would be expected. This however is in contradiction with the observed concave nature of the film curvature and the absence of a substrate curvature. On the contrary, the description of the phenomenon by means of a lateral distribution of the MD Burgers' vectors shows clearly its plastic nature. The origin of this distribution cannot be attributed to anomalous built-in characteristics of the substrates (such as residual off-cut or inhomogeneities of substrate BVs distribution). In fact, a concave curvature has been detected on the major part of the analyzed samples independently of the region of the wafer the samples were cut from. On the contrary, because the film curvature appears for the first time dramatically only in compositionally graded layers, we believe that the BULD must be connected to the presence of the vertical misfit gradient. This suggests that in graded buffers there are particular mechanisms of MD nucleation and/or MD multiplication which lead to the observed selection of BVs. Unfortunately both these mechanisms are not well understood even in uniformly strained epilayers so that we cannot give a full explanation.

However, the long range coherence of the curvature implies that the mechanism of BV selection must involve a characteristic length which is also macroscopic. The most natural choice for such a length is the glide length of MDs. Indeed graded buffers are especially designed to give long MD glide lengths: MDs in graded buffers have a reduced interaction due to their depth distribution and this fact allows them to reach probably an elongation up to several mm.[21] Furthermore the glide of MD leads to the required transport of the BV information over macroscopic distances. This hypothesis would also explain why so far the film curvature has been observed only for graded buffer layers and, to our knowledge, never reported in single layers where the glide lengths of MDs are much shorter.

The asymmetry of curvature in SB, i.e, much larger curvature along [110] than along $[1\bar{1}0]$, [see item (b)] is most probably connected with the well known asymmetry of MD nucleation along ⟨110⟩ directions in III–V semiconductors.[22,23] However, the ultimate reason for the much more symmetric curvature on LB compared to SB cannot be explained without a more detailed understanding of the process which leads to BULD.

Lattice curvature in a series of $In_xGa_{1-x}As$ buffer layers grown on well oriented [001] GaAs substrates has been shown for the first time. The main features of the phenomenon have been described on the basis of a lateral distribution of the Burgers' vectors and of reduced MD interaction. Nevertheless, a full comprehension of the driving force generating these tilts is not yet reached and further experimental investigations are necessary. We believe however that, similarly to the case of tilts on off-cut substrates, its understanding will give insight into mechanisms of MD formation in graded buffer layers.

Acknowledgment: The RSMs were collected at ESRF within the public user program.

[1] E. A. Fitzgerald, Y. H. Xie, M. L. Green, D. Bransen, A. R. Kortan, J. Michel, Y. J. Mii, and B. R. Weir, Appl. Phys. Lett. **59**, 811 (1991).

[2] F. K. LeGoues, B. S. Meyerson, and J. F. Morar, Phys. Rev. Lett. **66**, 2903 (1991).

[3] J. Tersoff, Appl. Phys. Lett. **62**, 693 (1993).

[4] Y. H. Xie, E. A. Fitzgerald, and P. J. Silverman, Mater. Sci. Eng., B **30**, 20 (1995).

[5] R. Beanland, D. J. Dunstan, and P. J. Goodhew, Adv. Phys. **45**, 87 (1996).

[6] A. Sacedon, F. Gonzalez-Sanz, E. Calleja, E. Munoz, S. I. Molina, F. J. Pacheo, D. Araujo, R. Garcia, M. Lourenco, Z. Yang, P. Kidd, and D. Dunstan, Appl. Phys. Lett. **66**, 3334 (1995).

[7] E. A. Fitzgerald and S. B. Samavedam, Thin Solid Films **294**, 294 (1997).

[8] D. J. Dunstan, H. G. Colson, M. A. Lourenco, A. Sacedon, F. Gonzalez-Sanz, L. Gonzalez, Y. Gonzalez, R. Garcia, D. Gonzalez, F. J. Pacheco, and P. J. Goodhew, J. Cryst. Growth **169**, 649 (1996).

[9] G. Salviati, L. Lazzarini, C. Ferrari, P. Franzosi, S. Milita, F. Romanato, M. Berti, M. Mazzer, A. V. Drigo, M. R. Bruni, M. G. Simeone, and N. Gambacorti, Scanning Microsc. **8**, 943 (1994).

[10] A. Bosacchi, A. C. De Riccardis, P. Frigeri, S. Franchi, C. Ferrari, S. Gennari, L. Lazzarini, G. Salviati, A. V. Drigo, and F. Romanato, J. Cryst. Growth **175/176**, 1009 (1997).

[11] B. Lee, J. H. Baek, J. H. Lee, S. W. Choi, S. D. Jung, W. S. Han, and E. H. Lee, Appl. Phys. Lett. **68**, 2973 (1996).

[12] B. H. Muller, R. Lantier, L. Sorba, S. Heun, S. Rubini, M. Lazzarino, A. Franciosi, E. Napolitani, F. Romanato, A. V. Drigo, L. Lazzarini, G. Salviati, J. Vac. Sci. Technol. (to be published).

[13] P. M. Mooney, F. K. LeGoues, J. Tersoff, and J. O. Chu, J. Appl. Phys. **75**, 3968 (1994); R. S. Goldman, H. H. Wieder, and K. L. Kavanagh, Appl. Phys. Lett. **67**, 344 (1995).

[14] F. K. Legoues, P. M. Mooney, and J. O. Chu, Appl. Phys. Lett. **62**, 140 (1993).

[15] J. M. Kang, C. S. Son, Moo-Sung Kim, Y. Kim, S. K. Min, and C. S. Kim, Appl. Phys. Lett. **67**, 641 (1995).

[16] A. Carnera and A. V. Drigo, Nucl. Instrum. Methods Phys. Res. B **44**, 357 (1990).

[17] L. C. Feldmann, J. W. Mayer, and S. T. Picraux, *Material Analysis by Ion Channeling* (Academic, New York, 1982).

[18] M. Mazzer, A. Carnera, A. V. Drigo, and C. Ferrari, J. Appl. Phys. **68**, 531 (1990).

[19] The sign of tilt depends on the average orientation of b_3 and on the choice of the MDs direction that here is: $\xi=-x_j$.

[20] Assuming the presence of only 60° MDs, it follows that $n_j^m=(\Delta f^m-\Delta\epsilon_{ii}^m)/|b_i|$, Δf^m, and $\Delta\epsilon_{ii}^m$ are the misfit and the residual parallel strain component at the mth interface, respectively.

[21] M. J. Matragrano, D. Ast, G. P. Watson, and J. R. Shealy, J. Appl. Phys. **79**, 776 (1996).

[22] K. L. Kavanagh, M. A. Capano, L. W. Hobbs, J. C. Barbour, P. M. J. Maree, W. Schaff, J. W. Mayer, D. Pettit, J. M. Woodall, J. A. Stroscio, and R. M. Feenstra, J. Appl. Phys. **64**, 4843 (1988).

[23] B. A. Fox and W. A. Jesser, J. Appl. Phys. **86**, 2739 (1990).